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FAST ALGORITHMS FOR PARTIAL DIFFERENTIAL EQUATIONS ON ADVANCED COMPUTERS

Final Report AFOSR 86-0061

Thomas A. Manteuffel

INTRODUCTION.

This report will cover four areas of research. The first area is an analysis of preconditionings. We have examined the properties that a preconditioning must possess in order to yield an iterative method with convergence properties independent of the discretization parameters. The second area is an attempt to provide a framework for the construction of conjugate gradient methods. The third area of research is the analysis of the equations governing the transport of neutrally charged particles and the construction of iterative methods for the solution of discrete transport equations. The final area of research is supraconvergence which deals with accurately approximating the solution of partial differential equations on highly irregular meshes.

The first topic is very theoretical in nature but will have important implications to the practical choice of preconditionings. The second area is also theoretical in nature, but leads immediately to the development of new iterative methods. The third area builds on the analysis of the continuous operators to yield insight into the behavior of discrete approximations. The final goal of this third project is the development of efficient numerical methods for the solution of discrete transport equations on massively parallel machines. The final area of research will lead to more efficient solution of differential equations on irregular meshes.

1. ANALYSIS OF PRECONDITIONINGS

Uniformly elliptic partial differential equations in R^2, denoted here by

$$Au = f,$$

yield discrete linear systems of equations

$$A_h u_h = f_h,$$

with condition number

$$\kappa(A_h) = O(h^{-2}),$$

where h is a mesh parameter. Iterative methods for the solution of the discrete equations yield error bounds after m steps of the type

$$\|e_m\| \leq K \left(\frac{k-1}{k+1} \right)^m \|e_0\|$$

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where $k = Cond(A_h)$ or $Cond(A_h)^{\frac{1}{2}}$ depending on the implementation.

Preconditioning can be viewed as a linear rearrangement of the equations in an attempt to reduce the condition number. The discrete equation is replaced by

$$C_h A_h \underline{u} = C_h \underline{f}$$

where C_h is a nonsingular linear process. Classical splitting methods may be viewed from this perspective. For example, S.O.R. with optimal parameter (applied to appropriate systems) yields a preconditioning for which

$$Cond(C_h A_h) = O(h^{-1}).$$

Likewise, incomplete factorization techniques yield preconditionings with this same property. Although of the same asymptotic order as S.O.R., incomplete factorizations perform better on a wide class of problems because the absolute magnitude of the condition number is smaller.

It was shown by D'Yakanov [DY1], [DY2] and Gunn [GU1] that for a special class of self-adjoint uniformly elliptic operators it is possible to construct B_h such that

$$Cond(B_h^{-1} A_h) = O(1),$$

that is, the condition number of the preconditioned system is independent of the mesh parameter. Here B_h is the discretization of a 'nearby' uniformly elliptic operator, B. The error in the original problem can be reduced by a given factor in a fixed multiple of the work required to solve systems of the type

$$B_h \underline{u} = \underline{f}.$$

The multiple is independent of the mesh but depends upon how 'close' A is to B.

This result was exploited by Concus and Golub [CO1] and Widlund [WI1] who noticed that if A and B live on a rectangle and if B is separable, then the equation involving B_h can be solved using fast direct methods (cf. [SW1]). Practice has shown that these methods are of little use unless A is very 'close' to a separable B. The difficulty is that while $Cond(B_h^{-1} A_h)$ is independent of the mesh, for reasonable values of the mesh parameter h the magnitude of the condition is larger than that for other splittings, for example, incomplete factorization.

Multigrid may also be viewed as a preconditioning where C_h represents the process of cycling through the grids. For a wide class of problems, $Cond(C_h A_h)$ is not only independent of h, but very small.

Results. The methods of D'Yakanov and Gunn and multigrid methods satisfy the same asymptotic bounds on the condition number. Yet, in practice, their performance can differ greatly. An attempt to develop a theory that encompasses these methods and yields more precise measurements of the practicality of preconditioning was presented in a report by Faber, Manteuffel, and Parter [FA4]. This work developed the concept of equivalent operators on Hilbert spaces. Two operators A

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and B are said to be equivalent in norm on the subset D of the Hilbert space H if the ratio

$$||Ax||/||Bx||$$

is bounded above and below for every element $x \epsilon D$. Equivalence in norm yields $Cond(AB^{-1})$ bounded on an appropriate domain. For preconditioned systems it is more appropriate to examine $Cond(B^{-1}A)$ or to show that A^{-1} and B^{-1} are equivalent in norm. An important result in this report is that if A_h and B_h are a sequence of discrete approximations to A and B, then $Cond(B_h^{-1}A_h)$ is bounded independent of h only if $Cond(B^{-1}A)$ is bounded. Thus, the construction of preconditionings independent of the mesh must be based upon equivalent operators.

This report was the basis for two papers [MA5], [FA5] (attached). In the first, uniformly elliptic operators were examined. It was shown that if Ω is a sufficiently smooth region in R^2, then any two uniformly elliptic operators with the same homogeneous boundary conditions are equivalent on a dense subset of $L^2(\Omega)$. One interesting corollary of this result is that if A_h and B_h are finite element discretizations of uniformly elliptic operators using elements smooth enough to be in the domain of A and B, then A_h and B_h are uniformly equivalent; that is, they are equivalent and the bounds are independent of h. This implies that $Cond(A_h B_h^{-1})$ will be independent of the mesh. This will lead to bounds on the residual $r_m = Ae_m$ of the type

$$||r_m|| \leq K \left(\frac{k-1}{k+1}\right)^m ||r_o||$$

where $k = Cond(A_h B_h^{-1})$.

To obtain similar bounds on the error e_m it is necessary to examine $Cond(B^{-1}A)$. It was discovered that $Cond(B^{-1}A)$ is bounded if and only if A^* and B^*, the L_2-adjoints of A and B, have the same homogeneous boundary conditions. It is easy to construct examples of operators A and B where $Cond(AB^{-1})$ is bounded while $Cond(B^{-1}A)$ is not and conversely. This discovery negates the conventional wisdom of choosing B to be the leading part of A with the same boundary conditions.

The second paper, [FA5], extends the theory in [FA4] to cover the situation where A and B are operators from a Hilbert space $\mathcal{W}$ to another Hilbert space $\mathcal{V}$. This paper establishes in a more general context the same results as [MA5]. Finally, this paper examines the uniform equivalence of finite element approximations. Similar results are established for some standard finite difference approximations when Ω is a rectangle.

These two papers also examine equivalence of weak forms of the operators A and B. Here, however, the H_1 norm replaces the L_2-norm in the definition of equivalence. It was discovered that $C_{H_1}(B^{-1}A)$ (the H_1 condition number) and $C_{H_1}(AB^{-1})$ are both bounded if and only if A and B have Dirichlet boundary conditions on exactly the same portions of the boundary of Ω. Similar results hold for their discrete counterparts.

Future Research. These results imply that under very general hypotheses preconditioning the discrete approximation of a uniformly elliptic operator by the discrete approximation of *any* other uniformly elliptic operator with the appropriate boundary conditions will yield a condition number independent of the mesh. This result demonstrates that a mesh independent bound alone is not sufficient to yield a good preconditioning. A measure of the distance between operators has been suggested [FA5] but is of little practical value. Conversely, these results imply that preconditioning strategies that yield mesh independent condition numbers most likely approximate the inverse of some operator equivalent to A.

A long list of interesting questions arises, some of them theoretical and some with more practical application. The above results depend upon H_2 regularity (or H_1 regularity for the weak forms) and uniform ellipticity. One theoretical question is whether these results hold in the absence of regularity. Another question is how to choose the operator B so that $B^{-1}A$ has its spectrum in the right-half plane, a potentially important issue for nonself-adjoint operators. This would determine the type of iteration implemented and whether

$$k = Cond(B_h^{-1}A_h) \text{ or } Cond(B_h^{-1}A_h)^{\frac{1}{2}}$$

in the error bound above.

Of more practical interest would be the development of a measure of the distance between two elliptic operators that could be computed or at least well approximated *a priori*. This would yield a good approximation to $Cond(B_h^{-1}A_h)$ and allow one to accurately predict the work required to solve the discrete system.

Even more fruitful would be the examination of multigrid methods in this context. Recent work by Parter [PA1] on singularly perturbed Helmholtz type equations has shown that in some cases one can achieve a mesh independent condition number using partial multigrid methods. These methods keep the coarsest grid very fine and never completely solve the coarsest mesh. This leads one to believe that similar methods may be applied to other problems. The marriage of multigrid with iterative techniques may guarantee a mesh independent condition number for a much wider class of problems than those for which multigrid has been applied to date.

2. Conjugate Gradient Methods.

Since the introduction of the conjugate gradient method in 1952 by Hentenes and Stiefel [HE1] it has become a popular method for the solution of symmetric positive definite linear systems. During the 36 years since its introduction, many variants have been developed including the preconditioned conjugate gradient method and the conjugate residual method.

Efficient generalizations of the conjugate gradient method to nonself-adjoint linear systems, other than forming the normal equations, were sought but never found. In the early 80's work by Faber and Manteuffel laid to rest this question by establishing both necessary and sufficient conditions for the existence of a short

term conjugate gradient method [FA1], [FA2]. In brief, given a linear system A and a preconditioning C it is possible to construct a three term conjugate gradient method optimal in the innerproduct norm $||x||_B^2 = \langle Bx, x\rangle$ if and only if *i)* CA has fewer than three distinct eigenvalues, or *ii)* CA is B-normal (1). The second criteria is an extension of the standard definition of normality. Here normality is measured with respect to the inner product $\langle B\cdot, \cdot\rangle$. The criteria is equivalent to the expression

$$BA = \alpha B + \beta A^* B$$

where A^* is the standard adjoint. This work showed that the conjugate gradient method could be extended, but only to a relatively small class of nonself-adjoint linear systems.

Results. The paper by Ashby, Manteuffel and Saylor [AS1] (attached) is an attempt to use the theory developed in [FA1] and [FA2] to provide a structure that includes all conjugate gradient methods. This structure not only shows how many variants of the conjugate gradient method are really different implementations of the same method, but also unambiguously determines the set of linear systems for which the method is applicable. Finally, this theory leads to the easy development of new methods. In fact, this paper introduces several new variants of the conjugate gradient method.

Future Research. The same principles have been applied to a much broader class of methods known as Projection Methods which include the conjugate gradient methods and are applicable to nonself-adjoint linear systems. Recent work by Joubert and Manteuffel [JO1] has established the beginnings of a theoretical framework for these methods. Future research will include expanding these results and examining several new methods exposed by this theory.

3. Multigrid Methods for Transport Theory

Mathematical models of radiation transport in optically dense materials are a fundamental part of many weapons codes. Similar problems arise in nuclear reactor design and analysis, satellite electronics shielding, radiation detector design and dosimetry, radiation therapy planning, and radiation effects on materials. Although two and three dimensional anisotropic models are of great interest, even the one dimensional model of transport in slab geometry presents formidable difficulties. This is because the equations governing transport become nearly singular on a subspace of large dimension in optically dense material, that is, when the mean free path between particle collisions is small compared to the physical dimensions. This is further complicated in that the subspace contains the functions of lowest frequency in space.

To be more precise, consider the equation governing neutron transport with isotropic scattering in a slab geometry,

$$\mu \frac{\partial}{\partial x} u(\mu, x) + u(\mu, x) = \frac{\gamma}{2} \int_{-1}^{1} u(\mu, x) d\mu + q.$$

Here, u is the particle density at spatial position x moving in direction characterized by angle θ, where $\mu = \cos\theta$, and q is the source term. This equation is to hold for $x\epsilon(-a,a)$ with boundary conditions

$$\begin{aligned} u(\mu,-a) &= b_1(\mu) \qquad 0 < \mu < 1 \\ u(\mu,a) &= b_2(\mu) \qquad -1 < \mu < 0. \end{aligned}$$

Here, γ is a positive constant with $\gamma \leq 1$. The space-like parameter x is scaled in terms of the number of mean free paths. Problems of interest generally involve $\gamma = 1$ and very large a.

The problem can be reformulated by defining the operators

$$L\cdot = \frac{1}{2}\int_{-1}^{1} \cdot d\mu$$

and

$$H_\mu = \mu\frac{\partial}{\partial x} + I,$$

yielding

$$H_\mu u = \gamma L u + q.$$

Inverting the transport operator H_μ yields

$$u = H_\mu^{-1}\gamma L u + H_\mu^{-1} q.$$

Applying L to this equation and making the substitutions

$$\phi = Lu, \; f = LH_\mu^{-1} q,$$

yields

$$\phi - (LH_\mu^{-1}\gamma)\phi = f.$$

The operator $K = (LH_\mu^{-1}\gamma)$ can be shown to be a compact self-adjoint operator on $L_2(-a,a)$ with $\|K\| \leq 1$ (cf. [WI2]). Notice that applying L eliminates the dependence on the angle μ. The equation above can be viewed as an integral equation of the second kind on $L_2(-a,a)$.

For very large a, a singular value decomposition of K yields singular vectors that are asymptotic to Fourier vectors.

$$v_k = \begin{cases} \cos(\eta_k x) & k \text{ odd} \\ \sin(\eta_k x) & k \text{ even} \end{cases}$$

where

$$\eta_k = k\pi + 0(\frac{k}{a}), \qquad \text{for} \qquad \frac{k}{a} << 1,$$

and singular values

$$\sigma_k = 1 - \delta_k (\frac{k\pi}{2a})^2 + O\left((\frac{k}{a})^3\right),$$

where $1/4 + \frac{1}{3\pi^2} \leq \delta_k \leq 1/4 + \frac{1}{\pi^2}$ [FA3] (attached).

It is often the case that the solution can be well described by frequencies for which $\frac{k}{a} << 1$. This implies that the operator $I-K$ is nearly singular on frequencies of interest.

The discrete analogue of this equation retains many of these properties and introduces greater difficulties. The operators H_μ and L are discretized on a (x, μ) grid. A popular technique, known as the S_N or discrete ordinates method [CA1], is to approximate H_μ by a difference formla in space and to approximate L by a quadrature formula in μ. Thus, the discrete K_h can be applied by computing $(H_{\mu_i})_h^{-1}\phi_h$ for a discrete set of angles μ_i and applying a quadrature rule to form $K_h\phi_h$.

In the past, these problems were solved by the simple splitting iteration known as the source iteration,

$$\phi_h^{i+1} = K_h\phi_h^i + f_h.$$

For large a, this iteration will converge very slowly. Recently, an observation that slow convergence occurs in problems that are basically diffusive has led to an algorithm called Diffusion Synthetic Acceleration (DSA) (cf. Larson [LA1], [LO1]),

$$(I - G_h)\phi_h^{i+1} = (K_h - G_h)\phi_h^i + f_h,$$

where $G_h = T_h^{-1}$ and T_h is the discrete form of the diffusion operator

$$Tu = -\frac{1}{3}\frac{\partial^2 u}{\partial x^2} + u$$

with u satisfying appropriate boundary conditions. The DSA iteration can be rearranged to yield

$$\phi_h^{i+1} = (T_h - I)^{-1}(T_h K_h - I)\phi_h^i + (T_h - I)^{-1} T_h f.$$

Thus, the iteration requires only the solution of a two-point boundary value problem and application of the operator K at each step.

Results. Recent work by Faber and Manteuffel [FA3] (attached) includes an analysis of the singular values and singular vectors of the operator K in the limit of large a. These results are used to show that the DSA iteration is successful because the first few singular vectors and singular values of the selfadjoint compact operator K are well approximated by the first few singular vectors and singular values of the compact operator G. Put in this perspective, $(I - G)$ is a good preconditioning for $(I - K)$. Further, simple iterative methods can be used to accelerate convergence of the DSA iteration. In fact, numerical experiments show that a conjugate gradient

iteration with DSA as a preconditioner can reduce the overall work by a factor of three even in the most simple cases.

The DSA algorithm is extremely effective for problems with isotropic or mildly anisotropic scattering, but it is ineffective for problems with highly anisotropic scattering, such as charged particle problems [MO1]. Furthermore, certain practical difficulties often arise in applying the DSA method with high-order-accurate spatial differencing schemes. Specifically, stability considerations require that the diffusion operator used in the DSA scheme be derived directly from the spatially-differenced S_N equations, and non-standard forms of the diffusion equation that are very costly to solve can be obtained [AL1].

In principal, multigrid methods are well suited to the solution of integral equations of the second kind. Because K is compact, for any $\epsilon > 0$ all but a finite number of the singular values of K are less than ϵ. Thus, $I - K$ looks like the identity plus a finite rank operator. In addition, the lowest frequency singular vectors are those associated with the largest singular values of K. Potentially, these vectors could be well approximated on a coarse grid.

For large a, however, all frequencies of interest may be associated with singular values of K very close to unity. This difficulty is compounded in forming the discrete analogue. If the spatial mesh size h is chosen fine enough to accurately describe the frequencies of interest, it may still be many mean free paths wide. For example, in applications in radiative transport, a may be on the order of 10^6 and the number of mesh points may be 10^3. Then h is on the order of 10^3 mean free paths wide. This yields a discrete equation in which well over half of the singular values of K_h are very near unity and, because of the discretization error, the smallest singular values of K_h are well away from unity. Thus, even if the lowest half of the frequencies are resolved on a coarser grid, the effective condition number of $I - K_h$ due to the remaining singular values is extremely large.

Simple source iteration is not adequate for eliminating the high-frequency errors that cannot be resolved on a coarse mesh. Certain block relaxation techniques have recently been developed [BO1] that effectively attenuate high-frequency errors regardless of the size of h. Furthermore, they have demonstrated that these relaxation schemes are effective regardless of the anisotropy of the scattering. Thus multigrid methods are more generally applicable than the DSA method.

Recently, we have developed a relaxation scheme on the (x, μ) grid that corresponds to line relaxation in μ with a variable shift [MA6]. We have shown that this yields a multigrid smoothing rate of 1/3 on the relevant singular vectors. Moreover, after relaxation the error is nearly independent of μ. Thus, a coarse grid correction need not involve μ. More precisely, an effective coarse grid error correction equation can be found using the observation that errors that remain after relaxation are nearly independent of μ. A scheme based on these observations is currently being implemented to prove its effectiveness. The scheme has been adapted to both upwind difference approximations and the more complicated linear discontinuous difference schemes.

Future Research. Most importantly, the scheme can be generalized to anisotropic

scattering and to higher dimensions. For isotropic scattering, shifted line relaxation in μ requires solving diagnonal block matrices perturbed by a rank one operator. This can be solved effectively by capacitance matrix methods (cf. [BU1]). In the anisotropic case, the same relaxation scheme involves solving a simple block system perturbed by a small number of rank one operators. Although slightly more complicated, these may also be solved by capacitance matrix methods. In two dimensions, line relaxation in μ becomes plane relaxation in two angle parameters (μ_1, μ_2). Again these involve only simple block matrices plus low rank perturbations.

The algorithm is simple and inherently parallel. First, the relaxation scheme is local in space. Also, if a Jacobi-like scheme is used, all lines can be relaxed simultaneously. If a Gauss-Siedel-type scheme is used where parallelism can be achieved by using a zebra-like ordering, every other line can be relaxed simultaneously. In addition, the coarse grids are essentially conventional diffusion equations which can be handled by standard parallel multigrid algorithms.

The ultimate goal of this project is the production of software for the solution of these problems. The successful algorithms will be implemented in two forms. One will be designed for the Cray X-MP and directed toward production problems at LANL. The second will be coded for the Connection Machine (CM2).

4. SUPRACONVERGENCE.

The classical approach to proving order of accuracy of difference schemes for differential equations is to examine the truncation error. If the difference scheme is stable then the order of accuracy is bounded by the order of the truncation error. Unfortunately, on highly irregular meshes the truncation error associated with many difference schemes is of lower order. For example, the second-divided difference has second-order truncation error on a uniform mesh, but only first-order truncation error on highly irregular meshes.

Much work has been done to alleviate this apparent disadvantage of irregular meshes. One approach is to assume that the mesh satisfies some smooth mesh function. Another approach is to use more complicated difference schemes, for example, operator implicit schemes.

Recent work by Manteuffel and White [MA1], [MA2] and Kreiss, Manteuffel, Swartz, Wendroff and White [KR1] shows that for many standard difference schemes the error is actually second-order accurate despite first-order truncation error. More precisely, consider the simple equation

$$y' = f,$$

together with appropriate boundary conditions. Let D be the second divided difference operator on the grid function y and consider the discrete equation

$$Dy = f.$$

The associated error equations can be written

$$D\underline{e} = \underline{t}$$

where $\underline{e}$ is the error and $\underline{t}$ is the truncation error. For irregular meshes, $||\underline{t}||_\infty = 0(\delta)$ where δ is the maximum mesh size. We know that

$$||\underline{e}||_\infty = ||D^{-1}\underline{t}||_\infty \leq ||D^{-1}||_\infty ||\underline{t}||_\infty .$$

Since $||D^{-1}||_\infty$ is bounded independently of δ, we may conclude that $||\underline{e}||_\infty = 0(\delta)$ as well. However, the inequality above is unnecessarily crude. It can actually be shown that $||\underline{e}||_\infty = 0(\delta^2)$ despite the fact that $||\underline{t}||_\infty = 0(\delta)$. This phenomena has been labeled supraconvergence [KR1].

It is clear that the standard stability/consistency proof is insufficient to detect supraconvergence. New tools have been developed that have led to the discovery that many schemes for ordinary differential equations and partial differential equations possess this property on highly irregular meshes. One important tool is to write the differential equation as a first-order system of equations using auxiliary unknowns, discretize the first-order system with simple difference schemes and then algebraically eliminate the auxiliary variables. This process, if done correctly, yields a compact-as-possible difference scheme on the original equation. Since the solution to the reduced equations is algebraically identical to the solution of the first-order system, it inherits any properties that the first-order system possesses.

Results. The theory of supraconvergence has been applied to higher-order ordinary differential equations with surprising results. It is quite simple to write a higher-order equation as a first order system and to then discretize this system using a second order accurate difference scheme. In [MA3] (attached), a calculus of difference operators is introduced. Auxiliary operators are constructed that allow for easy reduction of the discrete system to a discrete compact-as-possible system for the original equation. A more detailed paper [MA4] which is near completion shows that this process is essentially unique. The process yields second-order accurate difference schemes for any order ODE. The truncation error, however, is not second order on irregular meshes. In fact, for say a fourth order equation, the truncation error is $O(\delta^{-2})$, not only inconsistant but increasing as δ becomes small.

Boundary conditions for partial differential equations become especially transparent in the context of first-order systems. The algebraic reduction of the first-order system yields correct boundary conditions for the original equation. This important aspect of the research will have implications for choosing difference schemes to link composite grids.

Future Research. These same tools have produced results for partial differential equations. On tensor product meshes the extension is easy [MA2]. However, on more complicated meshes the problem is difficult.

A recent report [LE1] develops a class of compact-as-possible difference schemes for parabolic equations on time lines, but irregular spacial mesh. The class possesses second-order accuracy despite first-order truncation errors. This report also includes results on hyperbolic equations. We show that a class of conservative difference schemes are first-order accurate on irregular meshes despite inconsistent truncation error. These results are extended to the nonlinear wave equation.

The more compelling question of supraconvergence for elliptic equations on irregular meshes remains open. Current research that also involves Andrew B. White, Jr., in Los Alamos National Laboratory, Max Gunzberger at Carnegie-Mellon University and David Levermore of the University of Arizona is focusing on 9-point schemes on logically rectangular meshes and variable point schemes on triangular meshes. The main idea is to define auxiliary unknowns that are not necessarily associated with the nodes of the mesh, to form two different inner product spaces, one that includes the original unknowns and another that includes the auxiliary unknowns, and to determine the adjoints of the difference schemes in the respective inner products. If the truncation error can be conveniently decomposed into portions in the range and the null space of the adjoint, then the truncation error can be written as a product of the first-order system times terms of possibly higher-order plus terms in the null space. In this way schemes can be analyzed to see if they possess supraconvergence.

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